



# **9<sup>TH</sup> ANNUAL CONFERENCE OF THE METABOLOMICS SOCIETY**

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## GRAPE ISOPRENOIDS: AUTOMATED DATA ANALYSIS IN MORE THAN 500 SAMPLES

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Plant isoprenoids, which include metabolites like chlorophylls, carotenoids, tocopherols, among many others, have important functions *in planta*, with specific compounds being involved in photosynthesis, photoprotection, as hormone precursors, or in attraction of pollinators. In terms of human interest, they contribute not only to fruit appeal, but have also health beneficial properties (vitamins, antioxidants), making these compounds the target of many breeding efforts.

Carotenoids in particular are of interest in the case of grape since they are the precursors of norisoprenoids, aromatic compounds with importance in wine making.

The current study is part of a system-wide project focusing on the untargeted metabolomic analysis of grape.

In this study the isoprenoid profiling of more than 500 grape samples was done using HPLC-DAD. Hundreds of 3-dimensional data sets (Retention time x Wavelength x Response) were generated, showing the presence of multiple compounds with different UV-Vis spectra. Traditionally these data would be analysed by integrating peak areas at the wavelength of maximum absorption for each individual compound and chromatogram, an error-prone and cumbersome process. Further complicating factors include retention time shifts and coeluting compounds.

By using an automated pipeline based on Multivariate Curve Resolution (MCR) we were able to process all files simultaneously and to provide estimates of pure spectra, elution profiles, and accurate estimations of peak area for each of the analysed metabolites. Furthermore retention time correction and clustering allowed for the automated population of a data matrix containing peak areas for each detected compound (known and unknown) in each grape sample.

Preliminary results of the isoprenoid profiling in grapes will be presented.

Wehrens, R., Carvalho, E., Masuero, D., Juan, A. & Martens, S. High-throughput carotenoid profiling using multivariate curve resolution. *Analytical and Bioanalytical Chemistry* (in press) doi:10.1007/s00216-012-6555-9